Pentane

109-66-0 | DTXSID2025846

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 2.68

Global applicability domain: Inside

Local applicability domain index: 9.88e-01

Confidence level: 6.36e-01

Nearest Neighbors from the Training Set

Image not found
Pentane
Measured: 1.96
Predicted: 2.68

Image not found
Chloroform
Measured: 2.80
Predicted: 2.69

Image not found
2-Methylpropanenitrile
Measured: 2.87
Predicted: 2.60

Image not found
1-Nitropropane
Measured: 3.25
Predicted: 2.53

Image not found
Methyl tert-butyl ether
Measured: 2.58
Predicted: 2.53